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THE SPACE GROUP OF META TOLUIC ACID

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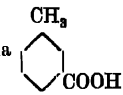
Plate VII

ABSTRACT. Goniometeric and X-ray study of single crystals of *m*-toluic acid shows that it belongs to monoclinic class. Crystallorgraphic data resulting from the above study is given by

$a=10\ 51$ Å, $b=8.01$ Å, $c=16\ 49$ Å, $\beta=92°\ 46.5'$.

Number of mocules per unit cell $=8$

Weissemberg photographs about crystallographic axes showed that (*hol*) planes are present when l is even and (*oko*) planes ae present when k is even. The crystal belongs to the space group C^5_{2h}—P_{2_1}/c, and so each one of the four asymmetric units is composed of two molecules.

m-Toluic acid or *m*-methylbenzoic acid has structural formula 

No goniometric or X-ray data are available for it. Single crystals of *m*-Toluic acid of suitable size were prepared by slow evaporation of the solution of the substance in ethyl alcohol. It gave prismatic crystals with six faces in one zone and having a tendency of elongation along this zone axis.

Goniometric measurement of the zone containing faces parallel to needle axis was made Rotation photograph about four selected zone axes were taken (Plate VII). Axial parameters thus got were further refined with the help of (00.12), (10.00), (00.14) reflections from Weissenberg goniometer photographs and are given below

$$a = 10.51\ \text{Å}$$
$$b = 8.01\ \text{Å}$$
$$c = 16.49\text{Å}$$
$$\beta = 92°46.5'$$

The interfacial angles measured and as calculated with the help of above axial parameters are given in Table I

The density of the crystals was determined by the floation method. The lighter liquid used was kerosene oil and the heavier carbon tetrachloride. Density

thus determined is 1.239 gm./cm^3. Thus the number of molecules comes out to be 8 per unit cell.

TABLE I

Indices of the faces	Measured interfacial angles	Calculated angles
$100 : 00\bar{1}$	92° 45′	β
$00\bar{1} : \bar{1}0\bar{2}$	34° 4′	37° 3.5′
$\bar{1}0\bar{2} : \bar{1}00$	50° 18″	50° 10.5′
$\bar{1}00 : 001$	92° 48′	β
$001 : 102$	37° 7′	37° 3.5′
$102 \cdot 100$	49° 58′	50° 10.5′

Zero layer line Weissenberg photographs along a and b axis and 1st layer line equi-inclination Weissenberg photograph about b axis were taken. On indexing them the following extinctions were observed.

(hol) planes absent for l odd.

(oko) planes absent for k odd.

No systemetic absence in the general planes (hkl).

The space group of the crystal is therefore C^5_{2h}—$P_{2_1/c}$. The number of asymmetric units per unit cell necessary for this space group is four, so two molecules form one asymmetric unit.

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PLATE VII

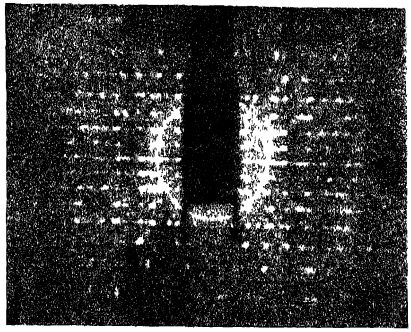

Fig 1.
About *c*-axis

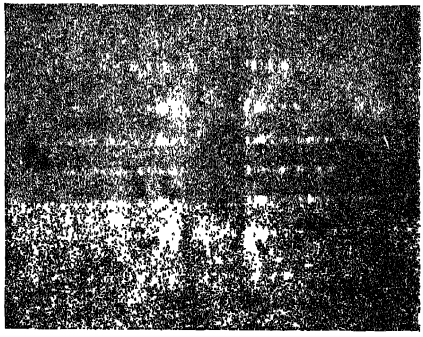

Fig 2.
About *b*-axis

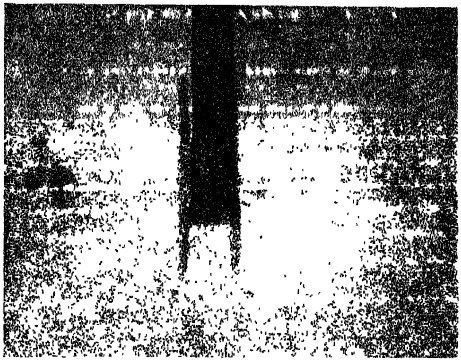

Fig 3.
About *a*-axis

Rotation photographs of *m*-toluic acid.